On the ground state of a completely filled lowest Landau level in two dimensions

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There exists a widely believed opinion, that the many-body ground state of a two-dimensional electron system at a completely filled lowest Landau level (the filling factor $\nu = 1$) is described by the so-called Hartree-Fock wave function, and that this solution is the unique, exact eigenstate of the system at $\nu = 1$. I show that this opinion is erroneous, construct an infinite number of other variational many-body wave functions, and discuss the properties of a few states which have the energy substantially lower than the energy of the Hartree-Fock state.

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The nature of the ground state of a system of two-dimensional (2D) interacting electrons in strong magnetic fields **B** was a subject of intensive investigations in the past years [1–24]. A great deal of attention was given to a partially filled lowest ($\nu < 1$) [1–16] or higher Landau levels ($\nu \gg 1$) [17–23]. The case of a completely filled lowest Landau level $\nu = 1$ was not adequately investigated in the literature. The only trial many-body wave function for this ν, the so-called Hartree-Fock solution,

$$\Psi_{HF}^{[N]} = \frac{1}{\sqrt{N!}} \det |\psi_{L_j}(\mathbf{r}_i)|, \quad L_j = 0, 1, \ldots, N-1, \tag{1}$$

was proposed in Ref. [24]. This is a Slater determinant, constructed from the lowest-Landau-level single-particle states

$$\psi_L(\mathbf{r}) = \frac{(z^*)^L}{\lambda\sqrt{\pi L!}} \exp(-zz^*/2), \tag{2}$$

and it is assumed that in the N-electron system the states $L = 0$ to $L = N-1$ are occupied by electrons. Here $z = (x + iy)/\lambda$ is a complex coordinate of an electron, $\lambda^2 = 2l^2 = 2\hbar c/eB$, l is the magnetic length, $L = 0, 1, 2, \ldots$ is the angular momentum quantum number, and $\hbar$, c, and e are the Planck constant, velocity of light and the electron charge, respectively. The wave function (1) is an eigenfunction of the kinetic energy operator, with the eigenenergy $E = N\hbar\omega_c/2$. It coincides with the Laughlin many-body wave function [6] at $\nu = 1$. The state (1) is characterized, in the thermodynamic limit, by a uniform 2D electron density $n_s(\mathbf{r}) = 1/\pi\lambda^2$ and the energy per particle [6]

$$\epsilon_{HF} = -\pi/2 = -1.57080 \tag{3}$$

in the B-independent energy units $e^2\sqrt{n_s}$.

There exists an opinion, that the Hartree-Fock many body wave function (1) is *the only one* possible solution of the problem at $\nu = 1$. Although this opinion is incorrect, it seems to be widely believed. The aim of this Letter is to show that the Hartree-Fock many-body wave function is not the only one possible trial wave function for the ground state of a 2DES at $\nu = 1$, and to demonstrate a number of other variational solutions of the many-body Schrödinger equation at $\nu = 1$, which have the energy substantially lower than the energy of the Hartree-Fock state.

I argue in three different manners.

The first argument is quite simple: in order to prove that the function (1) is not unique at $\nu = 1$, it is sufficient to present another explicit example of a trial wave function. Consider for instance the Wigner crystal many-body wave function [4],

$$\Psi_{WC}^{[N]} = \frac{1}{\sqrt{N!}} \det |\chi_{L=0}(\mathbf{r}_i, \mathbf{R}_j)|, \tag{4}$$

$$\chi_L(\mathbf{r}_i, \mathbf{R}_j) = \psi_L(\mathbf{r}_i - \mathbf{R}_j) e^{-i\pi \mathbf{r}_i \cdot (\mathbf{B} \times \mathbf{R}_j)/\phi_0}. \tag{5}$$

Here ϕ_0 is the flux quantum and $\mathbf{R}_j$ are points of a triangular lattice [4], distributed over the 2D plane with the average density n_s. This function depends on magnetic field and can be considered at $\nu = 1$. One can easily see that the projection of the Wigner crystal wave function onto the Hartree-Fock one is not unity. Expand the function $\chi_0(\mathbf{r}, \mathbf{R})$ in a set of the lowest-Landau-level eigenstates $\psi_L(\mathbf{r})$,

$$\chi_0(\mathbf{r},\mathbf{R}) \equiv \frac{1}{\sqrt{\pi}\lambda} e^{-zz^*/2 - ZZ^*/2 + z^*Z} = \frac{e^{-zz^*/2-ZZ^*/2}}{\sqrt{\pi}\lambda} \sum_{L=0}^{\infty} \frac{(z^*Z)^L}{L!} = \sum_{L=0}^{\infty} C_L(Z)\psi_L(\mathbf{r}), \tag{6}$$

where $C_L(Z) = Z^L \exp(-ZZ^*/2)/\sqrt{L!}$. Then, for the two-electron function (4) I get

$$\begin{aligned}
\Psi_{WC}^{[N=2]} &= \frac{1}{\sqrt{2!}} \det \left| \begin{array}{cc} \chi_0(\mathbf{r}_1,\mathbf{R}_1) & \chi_0(\mathbf{r}_1,\mathbf{R}_2) \\ \chi_0(\mathbf{r}_2,\mathbf{R}_1) & \chi_0(\mathbf{r}_2,\mathbf{R}_2) \end{array} \right| \\
&= \sum_{L_1=0}^{\infty} \sum_{L_2=0}^{\infty} C_{L_1}(Z_1) C_{L_2}(Z_2) \frac{1}{\sqrt{2!}} \det \left| \begin{array}{cc} \psi_{L_1}(\mathbf{r}_1) & \psi_{L_2}(\mathbf{r}_1) \\ \psi_{L_1}(\mathbf{r}_2) & \psi_{L_2}(\mathbf{r}_2) \end{array} \right| \\
&= \sum_{L_1=0}^{\infty} \sum_{L_2>L_1}^{\infty} \det \left| \begin{array}{cc} C_{L_1}(Z_1) & C_{L_2}(Z_1) \\ C_{L_1}(Z_2) & C_{L_2}(Z_2) \end{array} \right| \frac{1}{\sqrt{2!}} \det \left| \begin{array}{cc} \psi_{L_1}(\mathbf{r}_1) & \psi_{L_2}(\mathbf{r}_1) \\ \psi_{L_1}(\mathbf{r}_2) & \psi_{L_2}(\mathbf{r}_2) \end{array} \right|.
\end{aligned} \tag{7}$$

All the basis functions $\det|\psi_{L_j}(\mathbf{r}_i)|/\sqrt{2!}$ here are orthonormal. One of them (with $L_1 = 0$ and $L_2 = 1$) is the Hartree-Fock function (1). The projection

$$P \equiv \frac{|\langle WC|HF\rangle|^2}{\langle WC|WC\rangle\langle HF|HF\rangle} = \frac{\left|\det|C_{L_j}(Z_i)|\right|^2_{L_1=0,L_2=1}}{\sum_{L_1=0}^{\infty}\sum_{L_2>L1}^{\infty}\left|\det|C_{L_j}(Z_i)|\right|^2} \tag{8}$$

is evidently smaller than one. The same derivation can be easily performed at any N. In the thermodynamic limit $N \to \infty$ the projection (8) tends to zero, $P \to 0$.

Arbitrarily varying the vectors $\mathbf{R}_j$ (square lattice, other types of the lattice, random distribution), as well as taking the functions

$$\Psi_L^{[N]} = \frac{1}{\sqrt{N!}} \det|\chi_L(\mathbf{r}_i,\mathbf{R}_j)|, \tag{9}$$

with other angular momentum index L, one can easily get an infinite number of other explicit examples of many-body wave functions, different from (1).

The second argument is based on a standard degenerate perturbation theory. Consider the problem of N 2D electrons in a perpendicular magnetic field, in the presence of a neutralizing positive background, which has the form of a disk with the radius R and the charge density $+en_s$. The electroneutrality condition requires that $\pi R^2 n_s = N$. Assume that the total Coulomb energy of the system (electron-electron plus electron-background plus background-background interaction energy) can be considered as a perturbation. The ground state of the unperturbed problem is highly degenerate, therefore, one should use a degenerate perturbation theory. In the one-electron problem, one should search for a solution in the form $\Psi^{[N=1]}(\mathbf{r}) = \sum_{L=0}^{\infty} C_L \psi_L(\mathbf{r})$. This expansion contains all L-terms, from $L = 0$ to $L = \infty$. In the N-electron problem, one should write, similarly,

$$\Psi^{[N]}(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \sum_{L_1,\ldots,L_N}^{\infty} C_{L_1,\ldots,L_N} \frac{1}{\sqrt{N!}} \det|\psi_{L_j}(\mathbf{r}_i)|, \tag{10}$$

where, again, all L_i vary from $L_i = 0$ to $L_i = \infty$. The Hartree-Fock Slater determinant is the only one term in this expansion ($L_1 = 0$, $L_2 = 1$, ..., $L_N = N - 1$). Obviously, any variational solution of the many-body Schrödinger equation can be also searched for in the form of an arbitrary linear combination (10). Hence, the number of all possible trial wave functions (at any ν) is not one but infinite.

Finally (the third argument) I discuss the problem in the finite-cell geometry. In a number of papers (see e.g. Ref. [5]), the problem of a single 2D electron in a perpendicular magnetic field was considered in a finite rectangular cell ($0 \le x \le a$, $0 \le y \le b$), with periodic boundary conditions at the boundaries of the cell. According to [5], the "boundary condition requires that $ab/2\pi l^2$ be an integer m", and "there are m different single-electron states in the cell"

$$\phi_j(\mathbf{r}) = \left(\frac{1}{b\sqrt{\pi}l}\right)^{1/2} \sum_{k=-\infty}^{\infty} \exp\left[i\frac{(X_j+ka)y}{l^2} - \frac{(X_j+ka-x)^2}{2l^2}\right], \tag{11}$$

where $1 \le j \le m$ and $X_j = 2\pi l^2 j/b$. From this statement it follows that, at $\nu = 1$ the number of electrons per cell is exactly equal to the number of single-particle states, and therefore there exists only one possible way to construct the many-body wave function. Consider this argument in some more detail.

Consider a rigorous mathematical formulation of the single-electron problem in a finite-cell geometry. The wave function sought should satisfy the differential equation

$$\left[-\hbar^2\partial_x^2 + (-i\hbar\partial_y + eBx/c)^2\right]\phi(x,y) = 2mE\phi(x,y), \tag{12}$$

in the area $0 \le x \le a$, $0 \le y \le b$, and the boundary conditions

$$\phi(x,y=0) = \phi(x,y=b),\ \partial_y\phi(x,y=0) = \partial_y\phi(x,y=b),\ \text{ at all } 0 \le x \le a, \tag{13}$$

$$\phi(x=0,y) = \phi(x=a,y),\ \partial_x\phi(x=0,y) = \partial_x\phi(x=a,y),\ \text{ at all } 0 \le y \le b. \tag{14}$$

Standard substitutions, $\phi(x,y) = \varphi(x)\exp(ik_y y)$, $\xi = x/l + k_y l$, $\epsilon = 2E/\hbar\omega_c$, lead to the following equation for $\tilde{\varphi}(\xi) \equiv \varphi(x = l\xi - k_y l^2)$,

$$-\tilde{\varphi}''(\xi) + \xi^2\tilde{\varphi}(\xi) = \epsilon\tilde{\varphi}(\xi). \tag{15}$$

The second-order differential equation (15) has two independent solutions, e.g.

$$\Phi_1(\xi,\epsilon) = e^{-\xi^2/2}\left[1 + (1-\epsilon)\xi^2/2! + (1-\epsilon)(5-\epsilon)\xi^4/4! + \ldots\right] \tag{16}$$

and

$$\Phi_2(\xi,\epsilon) = e^{-\xi^2/2}\left[\xi + (3-\epsilon)\xi^3/3! + (3-\epsilon)(7-\epsilon)\xi^5/5! + \ldots\right]. \tag{17}$$

The total solution of eq. (12) is then written in the form

$$\phi(x,y) = e^{ik_y y}\left[C_1\Phi_1(x/l + k_y l,\epsilon) + C_2\Phi_2(x/l + k_y l,\epsilon)\right], \tag{18}$$

with two arbitrary constants C_1 and C_2. The boundary condition (13) requires that $k_y = 2\pi m/b$ with integer m. If the second boundary condition was imposed at infinity [$\phi(x = \pm\infty, y) = 0$] one would get a conventional solution of the problem, with $\epsilon_n = 2n + 1$, $n = 0, 1, \ldots$, and Landau eigenfunctions. In the finite-cell geometry, the boundary conditions (14) require that

$$\begin{array}{l}\{\Phi_1(k_y l,\epsilon) - \Phi_1(a/l + k_y l,\epsilon)\}C_1 + \{\Phi_2(k_y l,\epsilon) - \Phi_2(a/l + k_y l,\epsilon)\}C_2 = 0,\\ \{\Phi_1'(k_y l,\epsilon) - \Phi_1'(a/l + k_y l,\epsilon)\}C_1 + \{\Phi_2'(k_y l,\epsilon) - \Phi_2'(a/l + k_y l,\epsilon)\}C_2 = 0.\end{array} \tag{19}$$

Equations (19) determine the spectrum of eigenenergies $\epsilon = \epsilon_n(a/l, b/l)$, $n = 0, 1, \ldots$, and eigenfunctions of the problem (they are different from the Landau ones). Obviously, the boundary conditions do not restrict the number of eigenstates, and the single-particle spectrum remains unlimited.

One can easily verify, by means of a direct substitution, that the wave functions (11), proposed in [5], *do not satisfy* the boundary condition (14). Instead, they satisfy the boundary condition $\phi(x = a, y) = \exp(iay/l^2)\phi(x = 0, y)$. Hence, the functions (11) are not the eigenfunctions of the boundary-value problem (12)–(14), and the conclusion of Ref. [5] about a finite number of possible single-particle states in the considered problem is incorrect.

Now I present results of calculations of the energy of a few trial wave functions, different from the Hartree-Fock solution (1). I consider the functions Ψ_L, eq. (9), with $L = 0$ to 5, and with a triangular lattice of points $\mathbf{R}_j$, uniformly distributed over the 2D plane with the average density n_s. The states Ψ_L describe the properties of the system at all Landau-level filling factors $\nu \le 1$, continuously as a function of magnetic field. Like in [25], I calculate the Hartree energy exactly, in the thermodynamic limit, and the exchange-correlation energy approximately, at a finite number N of lattice points. Thus calculated energy per particle $\epsilon_L(N)$ is the upper limit to the true energy ϵ_L, $\epsilon_L < \epsilon_L(N)$ [25].

Figure 1 exhibits the energy $\epsilon_L(N)$ of the states Ψ_L, at $\nu = 1$, as a function of the number of lattice points N involved in calculation of the exchange-correlation energy. *All* the states Ψ_L, $L = 0, 1, \ldots, 5$, have the energy lower than the Hartree-Fock one. Some of them ($L = 1, 3, 4$ and 5) have the energy lower than the classical Wigner crystal [26]. The energy of the state $\Psi_{L=3}$ estimated with $N = 187$ lattice points, is more than 46% lower than the energy of the Hartree-Fock state. All the considered states are characterized by a strong overlap of the neighbor single-particle wave functions and by a uniform 2D electron density $n_s(\mathbf{r}) = 1/\pi\lambda^2$ at $\nu = 1$ (see for example, Figure 3 from Ref. [25]). Subsequent investigations of other trial wave functions (with other L and/or different symmetries of the lattice $\mathbf{R}_j$) may lead to even lower estimates of the ground state energy of the 2DES at $\nu = 1$. A huge variational freedom of the functions Ψ_L, which has been clearly demonstrated in this Letter, opens up wide possibilities to search for better approximations to the ground state, both at $\nu = 1$ and at all other ν.

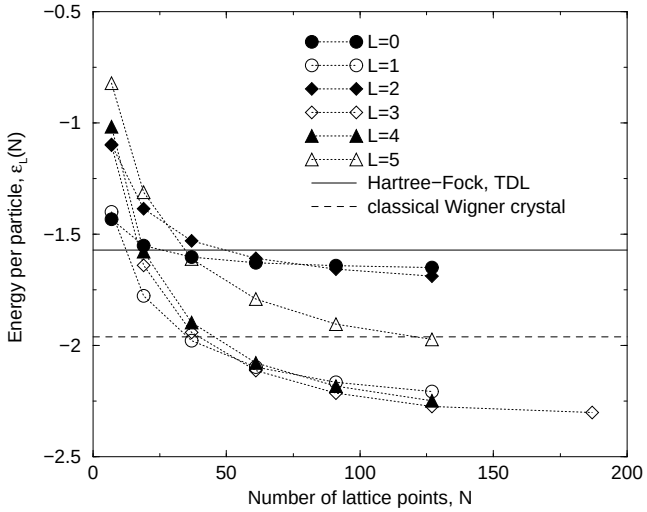

FIG. 1. Calculated energies $\epsilon_L(N)$ per particle of the states Ψ_L (in units $e^2\sqrt{n_s}$), as a function of the number of (triangular) lattice points N, for the states $L = 0$ to 5 at a completely filled lowest Landau level $\nu = 1$. The Hartree contribution is calculated in the thermodynamic limit, the exchange-correlation contribution – for a finite number N of lattice points. For comparison, the energies of the Hartree-Fock state (the thermodynamic limit, TDL) and of the classical Wigner crystal [26] are shown by solid and dashed lines respectively.

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